

Cryogenic Air Separation Using CHEMCAD Simulation

The study focuses on a cryogenic distillation air separation plant modeled entirely in CHEMCAD v8.0. Ambient air (50,000 Nm³/h) is compressed, cooled, and separated into nitrogen, oxygen, and argon using a multi-column cryogenic distillation system (HP, LP, crude argon, and pure argon columns). The work is simulation-based with industrially representative operating conditions.

CHALLENGE

Air separation plants require extremely high product purity, complex thermal integration, and precise vapor–liquid equilibrium control at cryogenic temperatures. Designing and validating such systems experimentally is costly and time-consuming. Additionally, commercial simulators may lack certain integrated industrial equipment (e.g., double columns, compressor after-cooling), making realistic modeling difficult. The challenge was to accurately simulate a full cryogenic air separation process in CHEMCAD while achieving industrial-grade purity levels for nitrogen, oxygen, and argon without process instability or simulation errors.

Academic Research*

- **Business Type:** Chemical Engineering Research / Process Simulation
- **Project Type:** Simulation-based design and performance evaluation of a cryogenic air separation unit (ASU).

SOLUTION

A detailed process model of a cryogenic air separation unit was developed using CHEMCAD simulation software. The model included air compression, staged cooling, a multistream main heat exchanger, expanders, and four distillation columns: a high-pressure column, a low-pressure column, a crude argon column, and a pure argon column. To overcome software limitations, integrated industrial equipment was represented using equivalent standalone units, and additional heat exchangers were introduced to simulate compressor after-cooling. Nitrogen backflow was strategically reused as a cooling utility to reduce external energy demand. Shortcut column design methods were first applied, followed by rigorous tray-by-tray distillation models to ensure separation accuracy.

**Adapted from ACS Omega 2024 9 (13), 15165-15174*

Organization / Authors: Hüseyin Berat Erdöl, Fatma İrem Şahin, and Nil Acaralı (Yıldız Technical University, Türkiye)

RESULTS

The CHEMCAD simulation ran successfully with no critical errors and only one non-limiting pinch warning in the main heat exchanger. High-purity separation of all major air components was achieved, validating both the thermodynamic models and process configuration. The simulation delivered stable operation across compressors, heat exchangers, and distillation columns while maintaining realistic industrial conditions.

KEY PRODUCT RESULTS

PRODUCT	PURITY	FLOW RATE (kg/h)
Liquid Oxygen (LOX)	99.49%	5,656.02
Liquid Nitrogen (LIN)	99.90%	4,664.66
Pressurized Gaseous Nitrogen (PGAN)	99.99%	25,524.49
Liquid Argon (LAR)	99.99%	699.94

TANGIBLE BENEFITS

- Demonstrated that CHEMCAD can reliably model complex cryogenic air separation systems.
- Achieved industrial-grade product purities (up to 99.99%) without experimental trials.
- Provided quantified mass flow benchmarks for nitrogen, oxygen, and argon production.
- Enabled evaluation of energy duties for compressors, heat exchangers, and distillation columns.
- Reduced design risk and development cost by validating process feasibility in simulation.
- Established a scalable simulation framework for future optimization, economic analysis, and sustainability studies.

REPRESENTATIVE DRAWINGS AND DATA

The original study includes key process flow diagrams and CHEMCAD simulation visuals, such as: Overall air separation unit process flow diagram; Pretreatment and compression section flow diagram; Cold box layout with multistream heat exchanger and distillation columns. These figures support understanding of thermal integration and column configuration. For portability, this case study summarizes the insights derived from those drawings rather than reproducing them directly.

TABLE 1 - Unit operation table for inlet and outlet streams of tower from the simulation program

tower type	trayed	tower type	trayed	tower type	trayed	tower type	trayed
number of stages	60	number of stages	30	number of stages	191	number of stages	22
1st feed stage	50	feed stage	12	feed stage	141	feed stage	7
2nd feed stage	58	draw stage for gas stream	19	column pressure (bar)	1.3	column pressure (bar)	1.3
column pressure (bar)	5.3	column pressure (bar)	1.4	calculated reflux ratio	35	calculated reflux ratio	6
calculated reflux ratio	1.2	calculated reflux ratio	11.6	estimated top temperature (°C)	-183.47	estimated top temperature (°C)	-193.42
estimated top temperature (°C)	-176.17	estimated top temperature (°C)	-192.59	estimated bottom temperature (°C)	-180.84	estimated bottom temperature (°C)	-183.15
estimated bottom temperature (°C)	-174.54	estimated bottom temperature (°C)	-180.07	calculated condenser duty (MJ/h)	-4266.95	calculated condenser duty (MJ/h)	-50.216
calculated condenser duty (MJ/h)	-9908.28	calculated condenser duty (MJ/h)	-57686.42			calculated reboiler duty (MJ/h)	50.210
calculated reboiler duty (MJ/h)	6190.27	calculated reboiler duty (MJ/h)	57946.25				

FIGURE 1 - Process flow diagram of the simulated air separation unit

